

Docusate sodium  
577-11-7 | DTXSID8022959

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.87	0.81	0.87	0.82	0.86	0.86

## Model Results

**Predicted value:** 3.81e-04 mol/L

**Global applicability domain:** Inside

**Local applicability domain index:** 2.52e-01

**Confidence level:** 4.76e-01

## Nearest Neighbors from the Training Set

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Cycloheptanecarboxylic acid, 1-  
((4-nitrophenyl)sulfonyl)-, 1-  
methylethyl ester

**Measured:** 8.50e-06

**Predicted:** 5.38e-05

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Cyclohexanecarboxylic acid, 1-  
((4-nitrophenyl)sulfonyl)-, 1-  
methylethyl ester

**Measured:** 1.32e-05

**Predicted:** 5.98e-05

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Cyclobutanecarboxylic acid, 1-  
((4-nitrophenyl)sulfonyl)-, 1-  
methylethyl ester

**Measured:** 1.74e-04

**Predicted:** 1.59e-04